

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101422\
 Data File : BP012132.D
 Acq On : 14 Oct 2022 11:49
 Operator : CG/JU
 Sample : N4976-06DL 2X
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 CB8Y1DL

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
 Title : SVOA CALIBRATION

Signal : TIC: BP012132.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.304	51	54	63	rVB	188593	251933	7.31%	0.677%
2	3.704	119	122	131	rBV	136040	204058	5.92%	0.549%
3	3.922	155	159	162	rVB4	17586	23250	0.67%	0.063%
4	4.016	172	175	179	rVB	14892	18957	0.55%	0.051%
5	4.463	247	251	262	rVB	102522	162037	4.70%	0.436%
6	5.151	363	368	375	rVB	26886	42967	1.25%	0.116%
7	5.410	409	412	420	rVB6	8787	18057	0.52%	0.049%
8	5.604	441	445	448	rBV4	6928	10396	0.30%	0.028%
9	5.775	472	474	482	rVB5	7572	12175	0.35%	0.033%
10	5.928	499	500	505	rVB4	4434	5155	0.15%	0.014%
11	6.122	530	533	539	rVB	9185	14935	0.43%	0.040%
12	6.445	582	588	592	rBV8	6748	13110	0.38%	0.035%
13	6.869	655	660	662	rBV6	5096	8711	0.25%	0.023%
14	7.016	678	685	697	rVB	130347	247692	7.18%	0.666%
15	7.110	699	701	706	rVB6	4198	6167	0.18%	0.017%
16	7.181	706	713	729	rBV	389329	670430	19.44%	1.803%
17	7.375	740	746	756	rBV	413476	673416	19.53%	1.811%
18	7.510	764	769	773	rVB8	5499	10910	0.32%	0.029%
19	7.698	798	801	805	rVB6	3560	5370	0.16%	0.014%
20	7.845	818	826	834	rBV	710664	1139151	33.04%	3.063%
21	7.934	834	841	848	rVB5	19137	52179	1.51%	0.140%
22	8.216	885	889	892	rVB3	8488	11777	0.34%	0.032%
23	8.328	902	908	913	rBV5	7882	14009	0.41%	0.038%
24	8.510	935	939	942	rBV5	5552	9849	0.29%	0.026%
25	8.563	942	948	957	rVV	349304	583843	16.93%	1.570%
26	8.634	957	960	967	rVB8	7745	14138	0.41%	0.038%
27	8.769	976	983	987	rBV4	12551	25589	0.74%	0.069%
28	8.839	989	995	997	rBV3	9125	15530	0.45%	0.042%
29	8.951	1010	1014	1018	rBV2	22361	32603	0.95%	0.088%
30	9.010	1018	1024	1036	rVV	424031	729443	21.16%	1.961%
31	9.169	1048	1051	1056	rBV6	4065	5822	0.17%	0.016%
32	9.216	1056	1059	1067	rVV10	4853	12048	0.35%	0.032%
33	9.369	1079	1085	1090	rBV	35696	58659	1.70%	0.158%
34	9.469	1096	1102	1110	rBV	68561	114459	3.32%	0.308%
35	9.592	1118	1123	1129	rVB7	11028	18601	0.54%	0.050%
36	9.657	1129	1134	1141	rVB10	7834	17079	0.50%	0.046%

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
 Title : SVOA CALIBRATION

37	9.734	1141	1147	1156	rBV	323994	564116	16.36%	1.517%
38	9.863	1160	1169	1175	rBV10	17290	42130	1.22%	0.113%
39	9.922	1175	1179	1181	rBV5	3982	5070	0.15%	0.014%
40	10.051	1198	1201	1206	rVB7	6721	12411	0.36%	0.033%
41	10.139	1212	1216	1218	rBV5	4292	7016	0.20%	0.019%
42	10.181	1218	1223	1233	rVB6	29105	70518	2.05%	0.190%
43	10.275	1233	1239	1248	rBV	527664	933813	27.08%	2.511%
44	10.339	1248	1250	1259	rVB9	17228	39269	1.14%	0.106%
45	10.439	1259	1267	1272	rBV2	38727	82658	2.40%	0.222%
46	10.563	1284	1288	1290	rBV4	5351	5979	0.17%	0.016%
47	10.604	1290	1295	1297	rVV2	26758	44489	1.29%	0.120%
48	10.651	1297	1303	1317	rVB	955955	1657018	48.06%	4.455%
49	10.798	1317	1328	1338	rBV	147335	323879	9.39%	0.871%
50	10.910	1343	1347	1355	rVV10	10996	27711	0.80%	0.075%
51	10.969	1355	1357	1361	rVV5	6418	8724	0.25%	0.023%
52	11.016	1363	1365	1370	rVB6	6320	7959	0.23%	0.021%
53	11.081	1372	1376	1382	rBV8	5350	9349	0.27%	0.025%
54	11.204	1393	1397	1400	rBV6	9901	13693	0.40%	0.037%
55	11.316	1411	1416	1418	rBV5	4773	6198	0.18%	0.017%
56	11.369	1420	1425	1431	rBV2	14056	25247	0.73%	0.068%
57	11.475	1432	1443	1444	rBV10	18085	42452	1.23%	0.114%
58	11.716	1479	1484	1495	rVB10	13996	36365	1.05%	0.098%
59	11.863	1501	1509	1514	rBV6	16166	35309	1.02%	0.095%
60	11.910	1515	1517	1522	rVB5	8309	12018	0.35%	0.032%
61	11.998	1524	1532	1536	rBV	42237	81751	2.37%	0.220%
62	12.039	1537	1539	1547	rVB7	10936	20956	0.61%	0.056%
63	12.186	1557	1564	1565	rBV5	11526	22125	0.64%	0.059%
64	12.233	1569	1572	1576	rBV4	14734	21993	0.64%	0.059%
65	12.275	1576	1579	1580	rBV3	10189	10539	0.31%	0.028%
66	12.375	1594	1596	1599	rBV3	5535	7005	0.20%	0.019%
67	12.422	1601	1604	1612	rBV5	12978	26871	0.78%	0.072%
68	12.657	1641	1644	1654	rVB6	19547	45298	1.31%	0.122%
69	12.875	1679	1681	1688	rVB7	14847	23301	0.68%	0.063%
70	13.086	1714	1717	1725	rVB10	15724	39569	1.15%	0.106%
71	13.386	1765	1768	1775	rBV	23095	31161	0.90%	0.084%
72	13.504	1785	1788	1791	rBV4	16013	18995	0.55%	0.051%
73	13.545	1792	1795	1799	rVB4	19207	26701	0.77%	0.072%
74	13.675	1814	1817	1821	rBV6	12863	21454	0.62%	0.058%
75	13.722	1821	1825	1827	rVV4	23078	33386	0.97%	0.090%
76	13.757	1828	1831	1836	rVB	42084	64501	1.87%	0.173%

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 Title : SVOA CALIBRATION

77	13.910	1851	1857	1863	rVB	926646	1305055	37.85%	3.509%
78	14.051	1878	1881	1884	rBV5	14195	22417	0.65%	0.060%
79	14.186	1898	1904	1918	rVB	1197183	1784748	51.76%	4.799%
80	14.304	1919	1924	1937	rVB	172951	296810	8.61%	0.798%
81	14.422	1939	1944	1950	rBV3	113736	164544	4.77%	0.442%
82	14.498	1950	1957	1964	rVB	1278854	1962883	56.93%	5.278%
83	14.722	1991	1995	2000	rBV	49781	85264	2.47%	0.229%
84	15.245	2080	2084	2089	rBV	101323	168516	4.89%	0.453%
85	15.492	2120	2126	2132	rBV	1519886	2139531	62.05%	5.753%
86	15.616	2142	2147	2152	rBV	310887	446093	12.94%	1.199%
87	15.751	2167	2170	2179	rVB3	50758	90358	2.62%	0.243%
88	16.010	2209	2214	2225	rBV	401017	628011	18.21%	1.689%
89	16.527	2295	2302	2307	rBV	210518	353281	10.25%	0.950%
90	16.792	2345	2347	2355	rVB2	44194	70592	2.05%	0.190%
91	17.257	2420	2426	2434	rBV	1511239	2226123	64.57%	5.986%
92	17.351	2437	2442	2452	rBV2	1604325	2333072	67.67%	6.273%
93	18.139	2573	2576	2584	rBV2	162612	251920	7.31%	0.677%
94	18.439	2624	2627	2630	rVB2	69913	77284	2.24%	0.208%
95	19.374	2783	2786	2793	rBV	122292	173563	5.03%	0.467%
96	19.592	2818	2823	2828	rBV	2266303	2953401	85.66%	7.941%
97	19.639	2828	2831	2839	rVB	390371	510643	14.81%	1.373%
98	21.345	3116	3121	3129	rBV	2225170	2833710	82.19%	7.619%
99	23.603	3499	3505	3517	rVB2	1673639	3447841	100.00%	9.271%
100	23.762	3526	3532	3543	rVB2	1539441	3102246	89.98%	8.341%

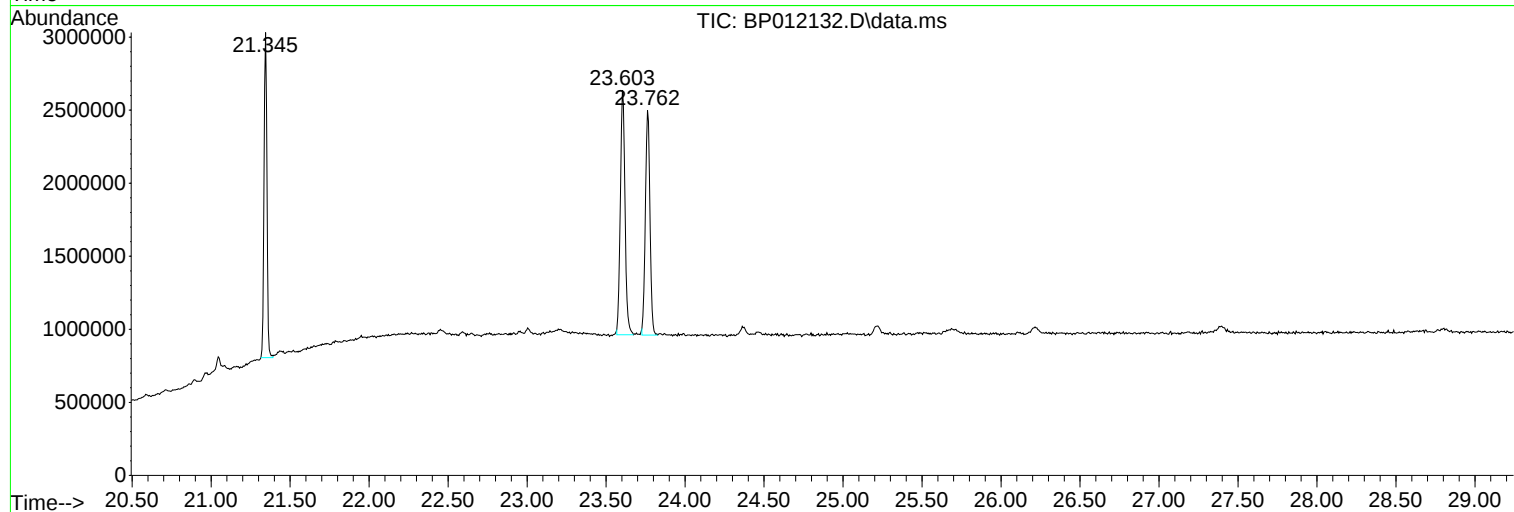
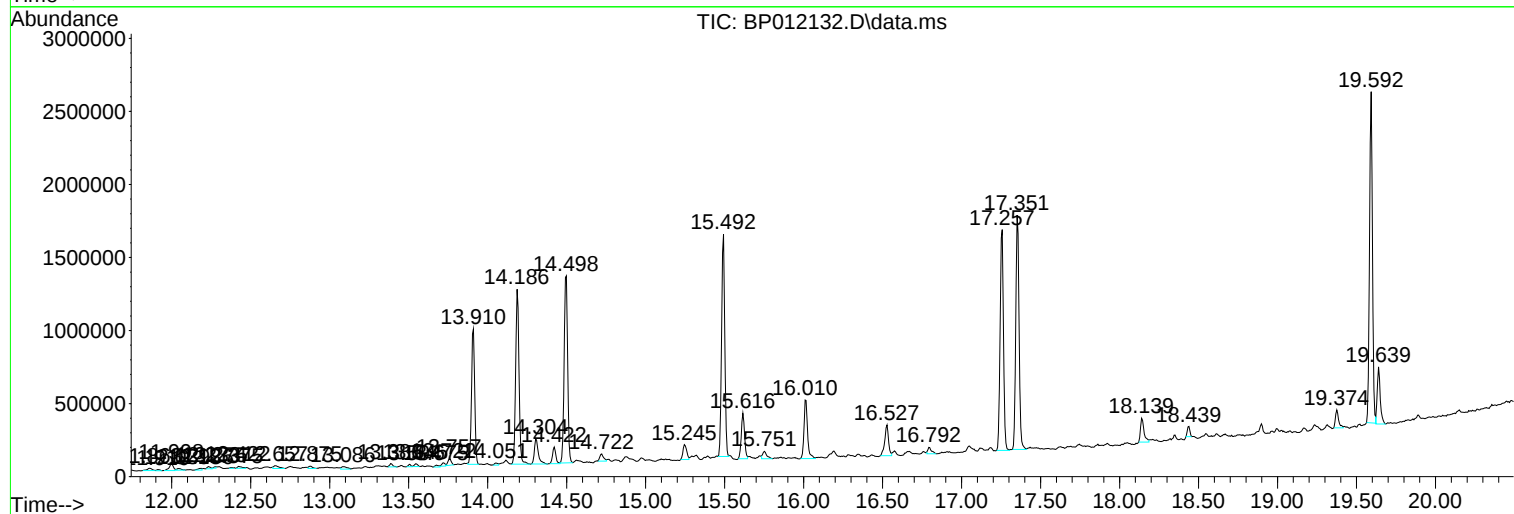
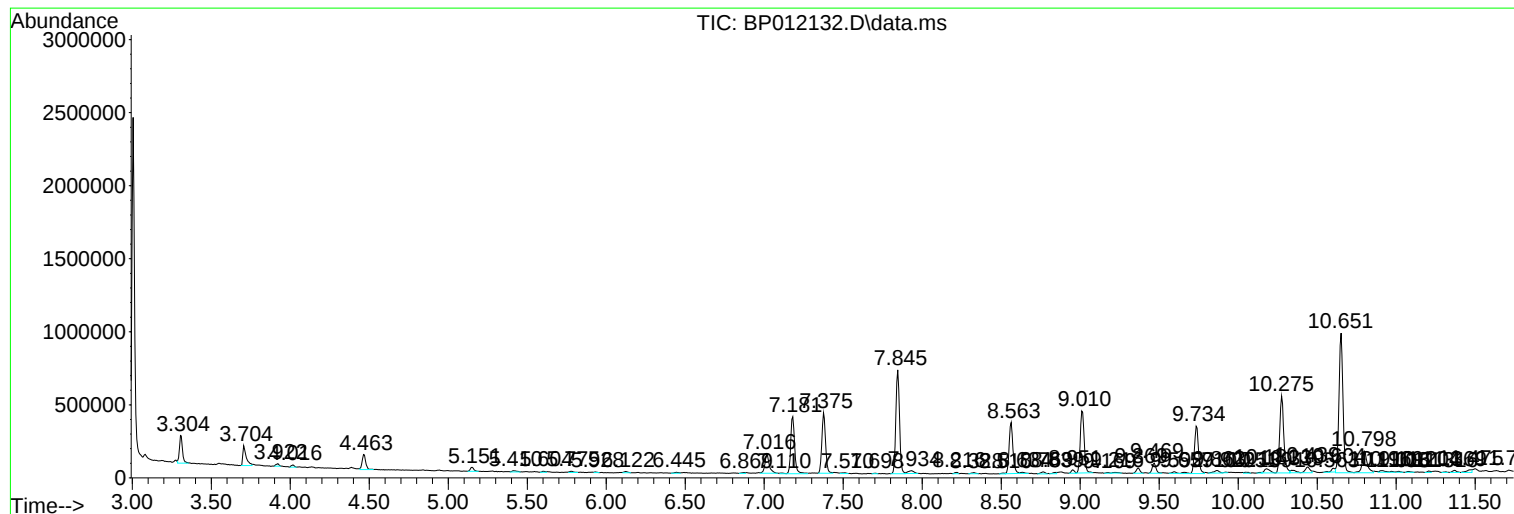
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P



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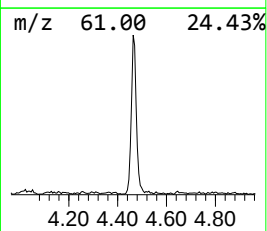
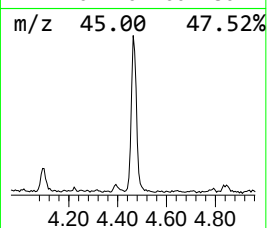
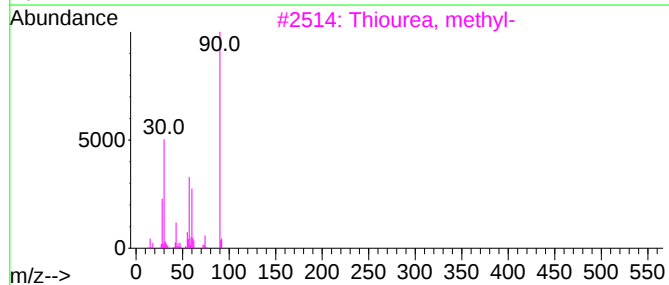
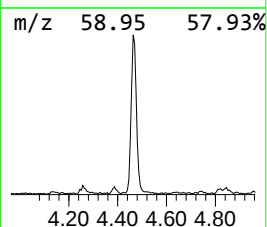
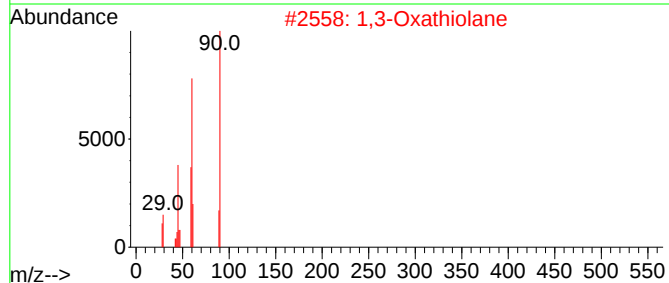
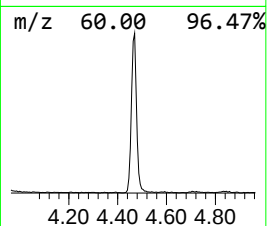
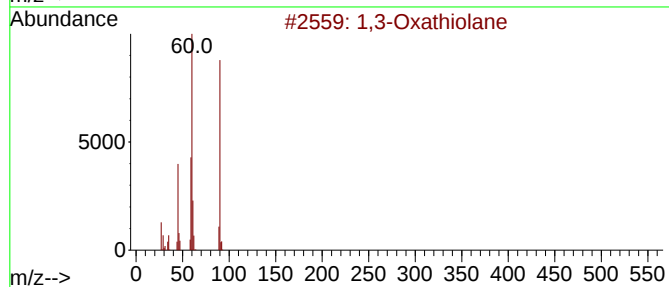
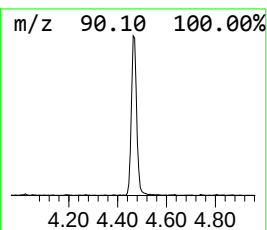
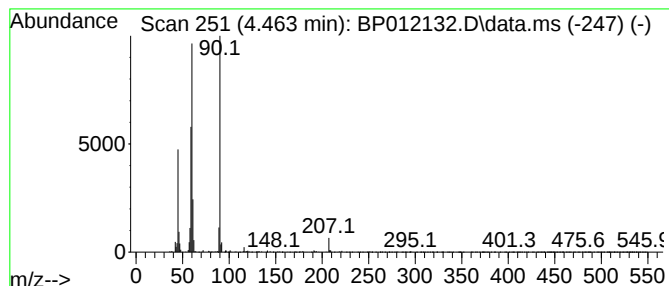
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1,3-Oxathiolane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.463	2.84 ng/ul	162037	1,4-Dichlorobenzene-d4	7.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Oxathiolane			90	C3H6OS	002094-97-5	91
2	1,3-Oxathiolane			90	C3H6OS	002094-97-5	78
3	Thiourea, methyl-			90	C2H6N2S	000598-52-7	50
4	3-Thietanol			90	C3H6OS	010304-16-2	42
5	Thiourea, methyl-			90	C2H6N2S	000598-52-7	36



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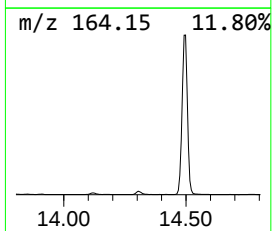
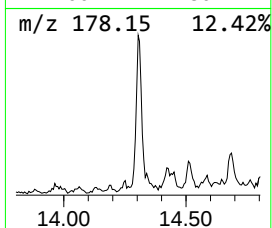
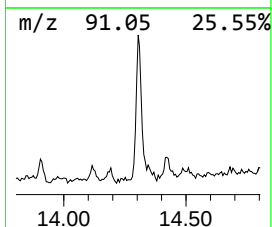
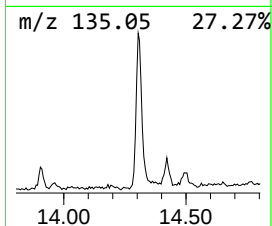
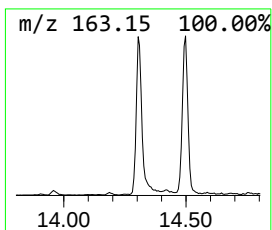
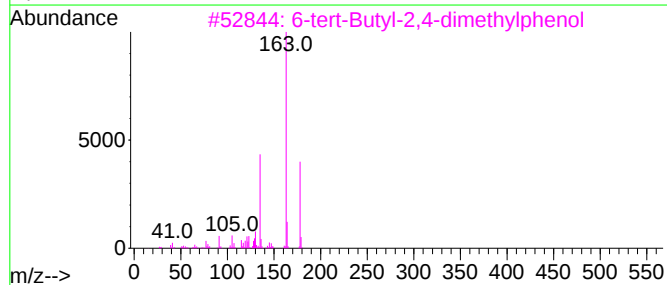
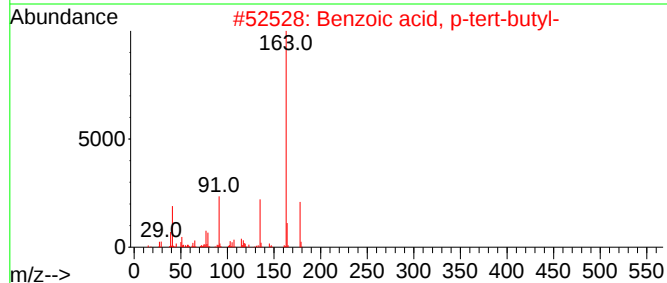
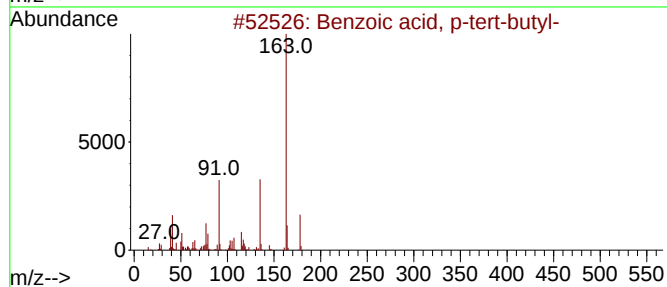
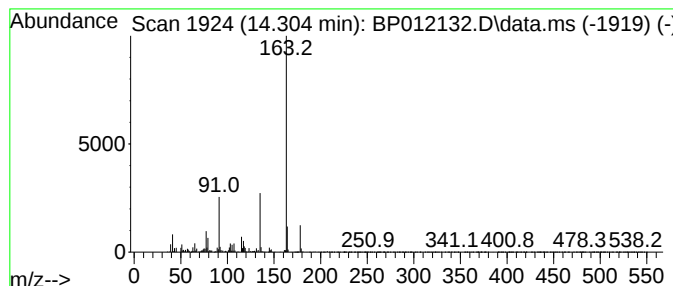
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzoic acid, p-tert-butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.304	3.02 ng/ul	296810	Acenaphthene-d10	14.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	93
3			6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	72
4			Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	72
5			Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	64



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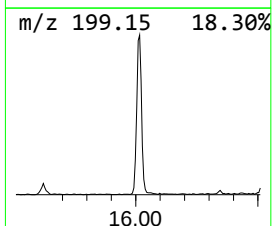
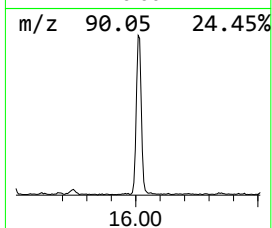
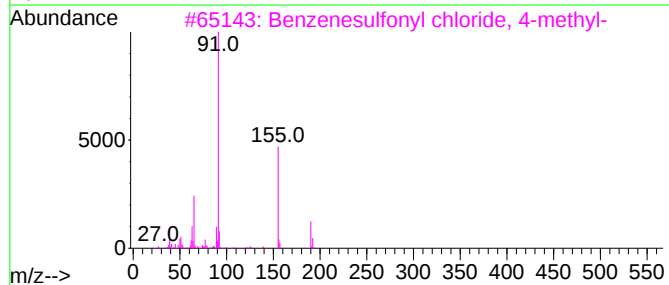
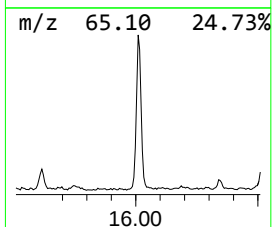
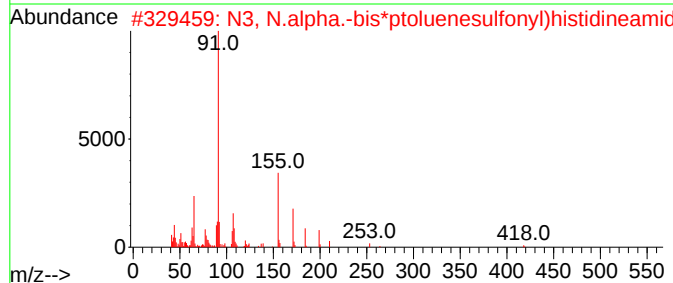
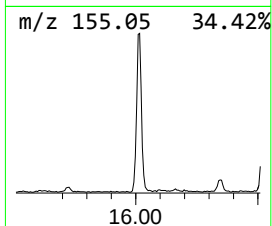
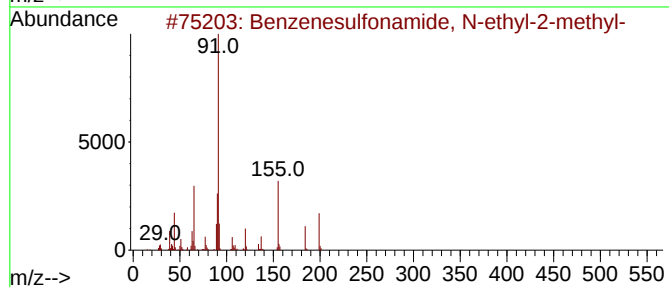
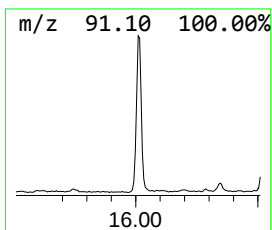
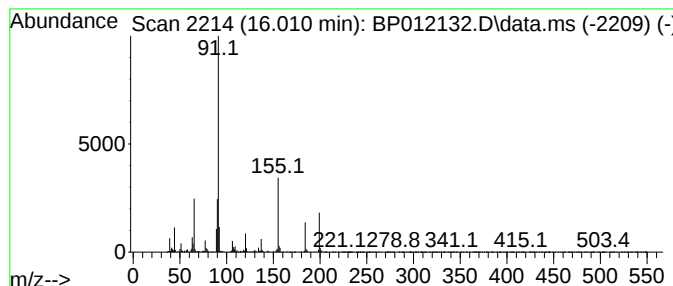
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzenesulfonamide, N-ethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.010	5.64 ng/ul	628011	Phenanthrene-d10	17.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N-ethyl-2-me...	199	C9H13NO2S	001077-56-1	95
2			N3, N.alpha.-bis*ptoluenesulfony...	462	C20H22N4O5S2	1000130-21-9	50
3			Benzenesulfonyl chloride, 4-methyl-	190	C7H7ClO2S	000098-59-9	50
4			benzenesulfonamide, 4-methyl-N-[-...	369	C16H19NO5S2	1000402-61-7	50
5			4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101422\
Data File : BP012132.D
Acq On : 14 Oct 2022 11:49
Operator : CG/JU
Sample : N4976-06DL 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB8Y1DL

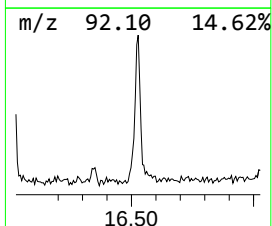
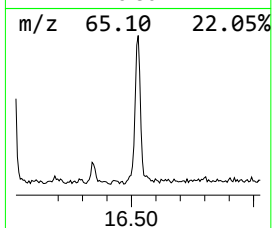
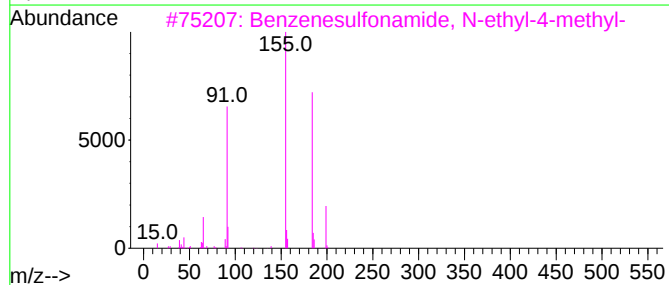
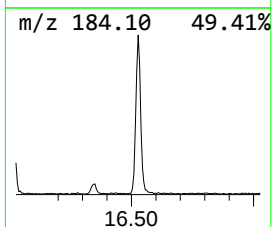
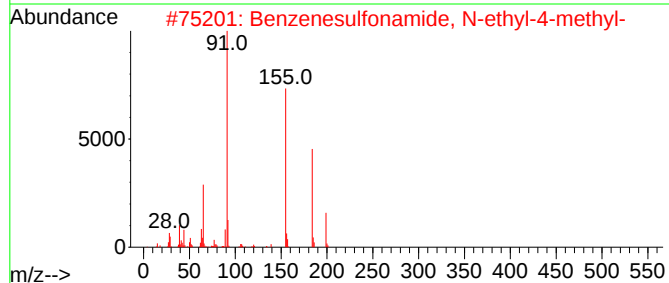
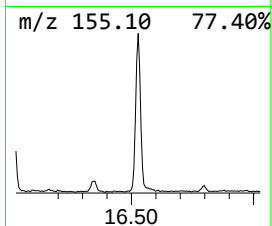
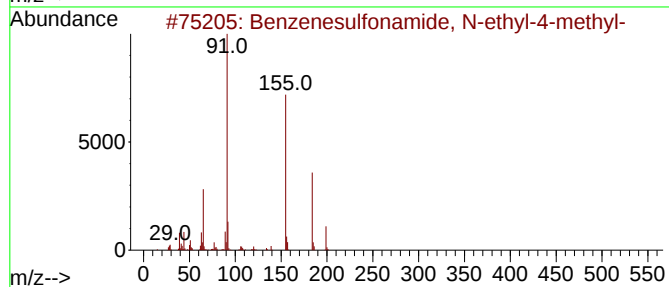
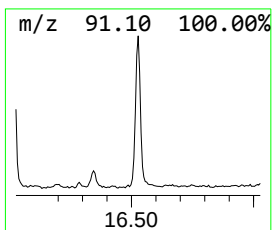
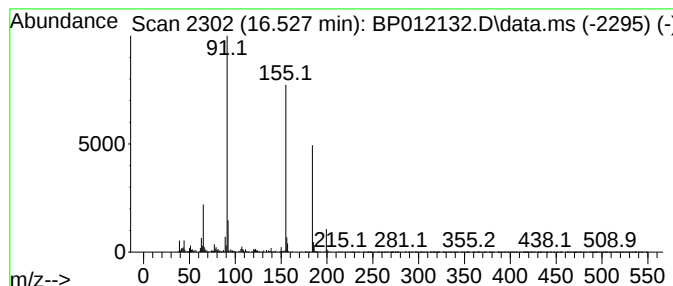
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzenesulfonamide, N-ethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.527	3.17 ng/ul	353281	Phenanthrene-d10	17.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	97
2			Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	93
3			Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	91
4			N-isobutyl-4-methylbenzenesulfon...	227	C11H17NO2S	023705-38-6	90
5			Benzene, 4-(ethylsulfonyl)-1-met...	184	C9H12O2S	007569-34-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101422\
Data File : BP012132.D
Acq On : 14 Oct 2022 11:49
Operator : CG/JU
Sample : N4976-06DL 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB8Y1DL

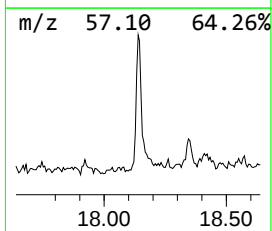
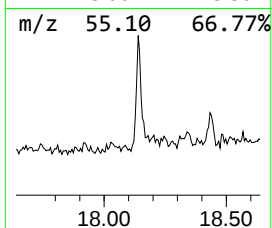
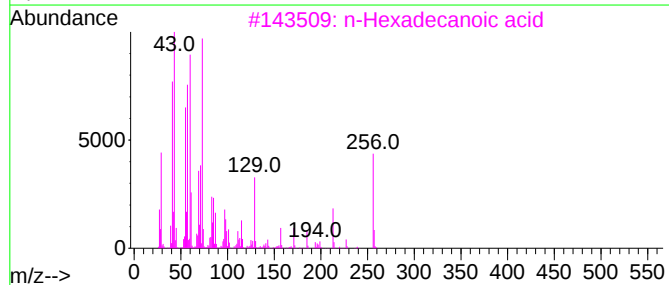
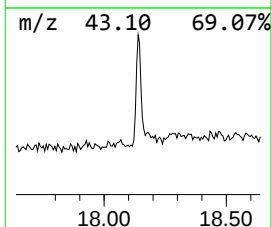
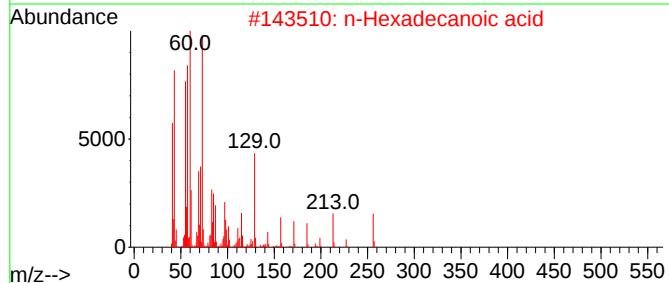
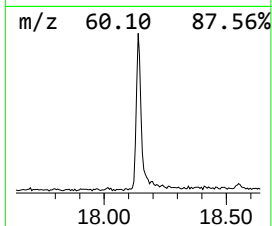
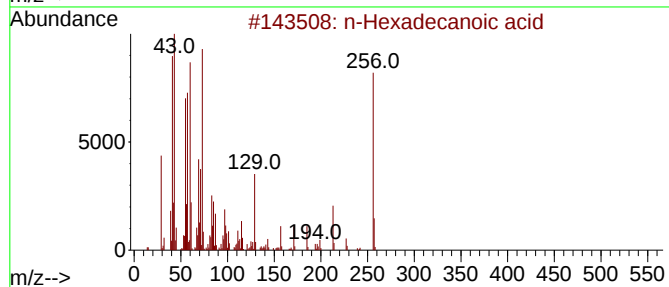
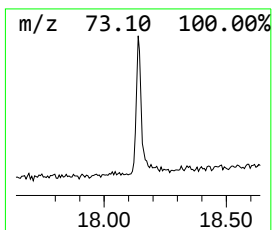
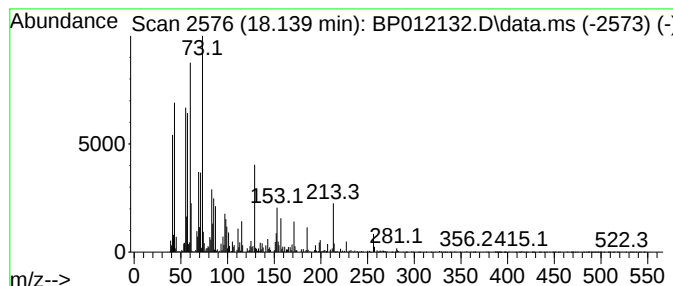
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.139	2.26 ng/ul	251920	Phenanthrene-d10	17.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
5			Tridecanoic acid	214	C13H26O2	000638-53-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101422\
Data File : BP012132.D
Acq On : 14 Oct 2022 11:49
Operator : CG/JU
Sample : N4976-06DL 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CB8Y1DL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP101122.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Oxathiolane	4.463	2.8	ng/ul	162037	1	7.845	1139150	20.0
Benzoic acid, p...	14.304	3.0	ng/ul	296810	3	14.498	1962880	20.0
Benzenesulfonam...	16.010	5.6	ng/ul	628011	4	17.257	2226120	20.0
Benzenesulfonam...	16.527	3.2	ng/ul	353281	4	17.257	2226120	20.0
n-Hexadecanoic ...	18.139	2.3	ng/ul	251920	4	17.257	2226120	20.0